

Delocalization Energy Retrieved from the Current Density Tensor Supporting Information

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Computational details

Molecular geometries of the isomers of benzene **16**, **102**, **185**, **187**, **199**, **213**, where numbers refer to ref.¹ (which in turn adopted the numbering of ref.²), have been obtained at the B3LYP/aug-cc-pVTZ level, starting from the output reported in the Supporting Information of ref.¹ Re-optimization led to no significant energy changes, but allowed defining the molecular symmetry, which turned out C_s in all cases, but benzene (D_{6h}). Molecules magnetic susceptibility has been computed by GIAO using the 175,974 points pruned grid available in Gaussian 09.

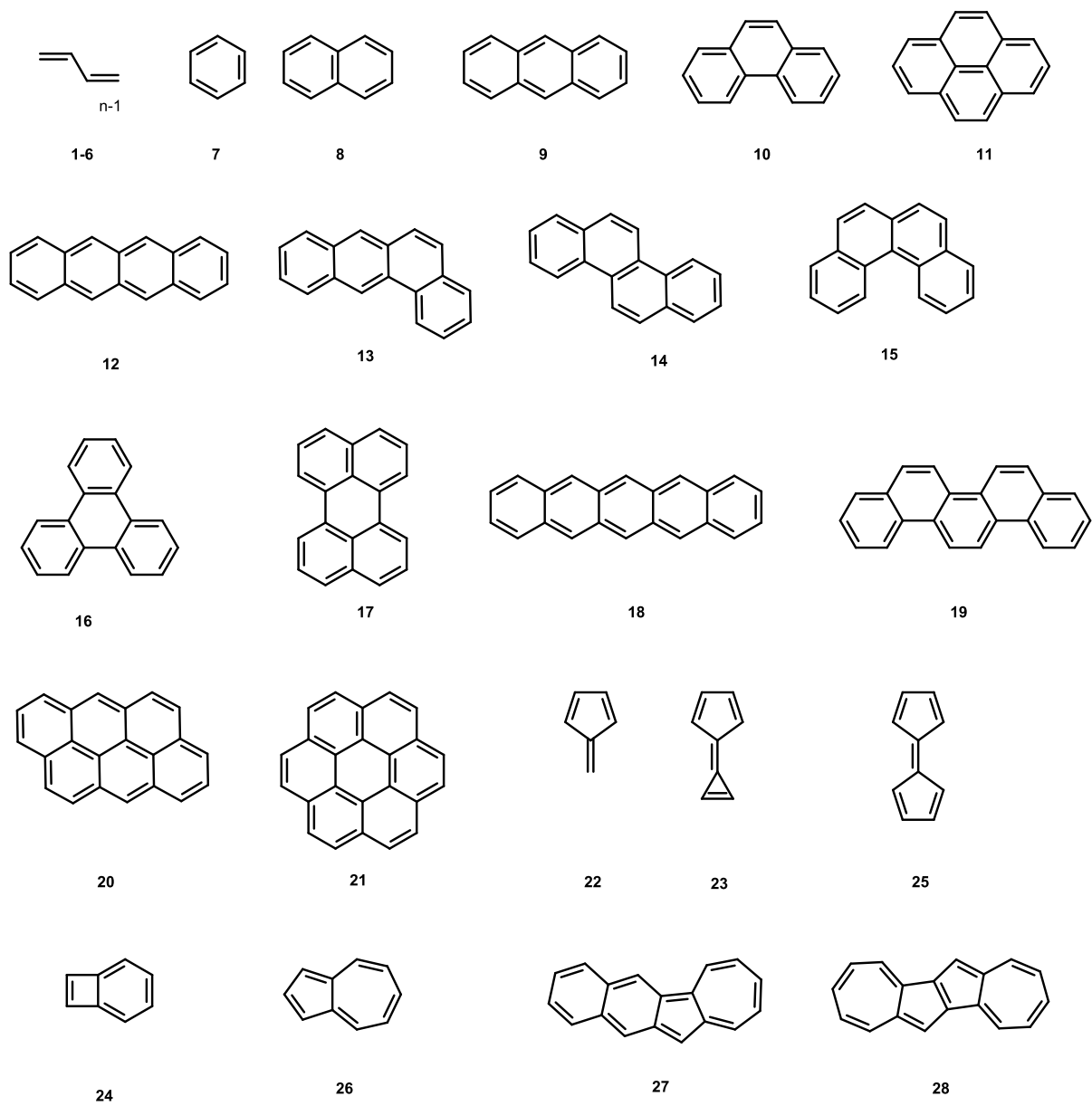


Figure S1: Sketches of the molecules listed in Table 1.

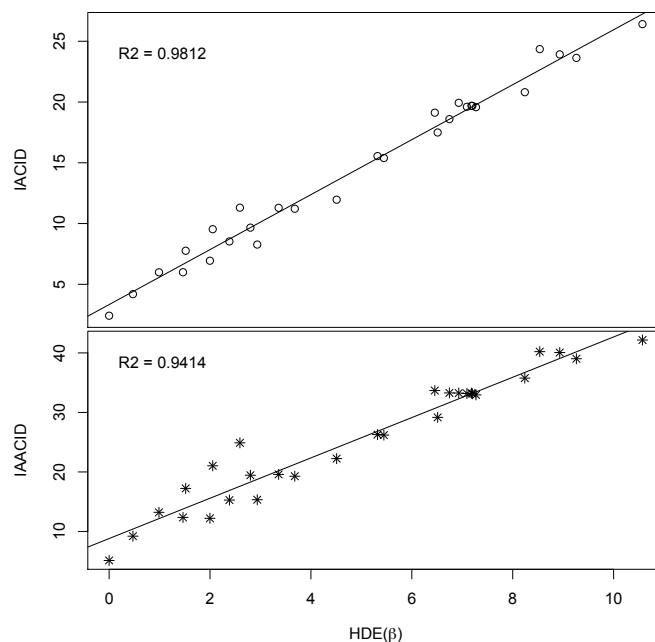


Figure S2: Scatter plots of integrated anisotropies versus the Hückel delocalization energies for the systems listed in Table 1.

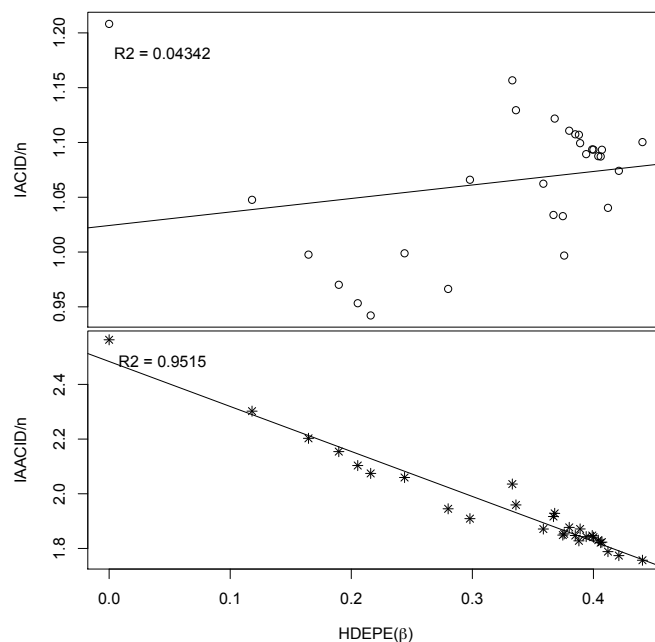


Figure S3: Scatter plots of normalized integrated anisotropies versus the Hückel delocalization energies per electron for the systems listed in Table 1; n is the number of π electrons, matching the number of C atoms in our set of molecules.

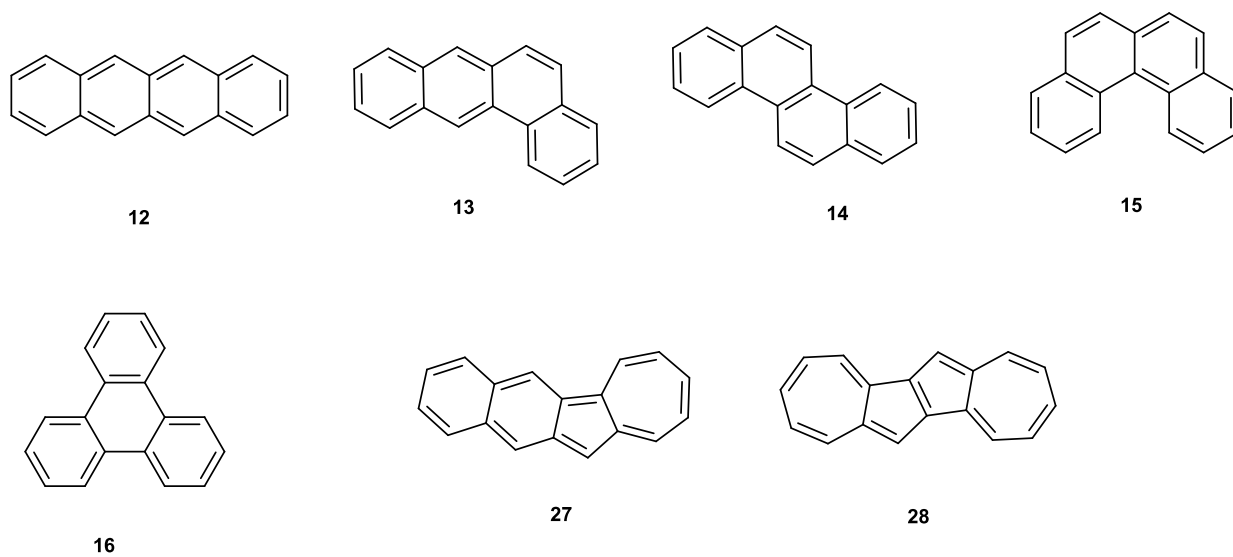


Figure S4: Sketches of the molecules listed in Table 1 with formula $C_{18}H_{12}$.

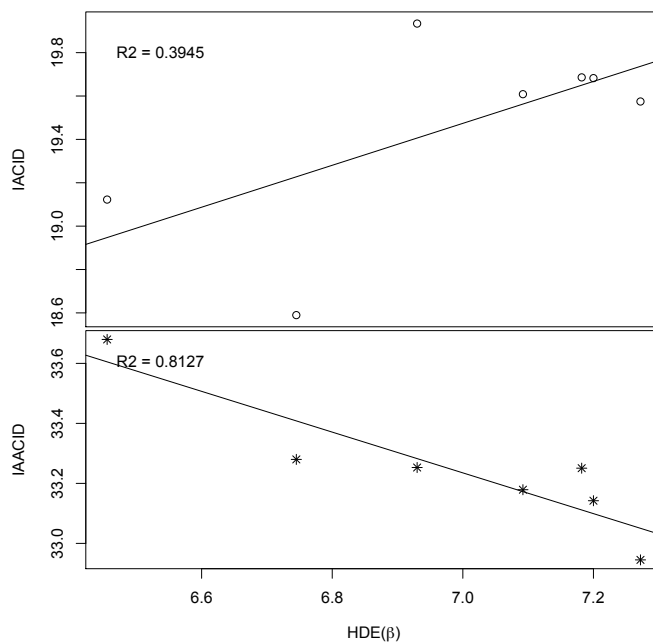


Figure S5: Scatter plots of integrated anisotropies versus the Hückel delocalization energies for the 7 $C_{18}H_{12}$ isomers among the molecules considered in the paper.

Table S1: Least squares coefficients and their standard errors for the four linear regressions discussed in the text.

x	y	parameter	ACID-based		AACID-based	
HDE	IACID IAACID	intercept	3.33	± 0.34	8.8	± 0.9
		slope	2.26	± 0.06	3.4	± 0.2
HDE	IACID IAACID (C ₁₈ H ₁₂ isomers)	intercept	12.71	± 3.74	38.0	± 1.0
		slope	0.97	± 0.54	-0.68	± 0.15
HDEPE	IACID/ n IAACID/ n	intercept	1.02	± 0.04	2.48	± 0.02
		slope	0.12	± 0.11	-1.65	± 0.07
HDE	Δ IACID Δ IAACID	intercept	-1.00	± 0.25	-0.3	± 0.2
		slope	-0.20	± 0.04	-1.81	± 0.03

Table S2: Results for the isomers of benzene computed as described in the Computational Details. Energies and integrated anisotropies in atomic units. Values of magnetizabilities in 10^{-30} J T⁻².

Isomer	IACID	IAACID	E	ξ_{iso}	$\Delta\xi$	ξ_1	ξ_2	ξ_3
16	6.84	12.69	-232.33729	-932.1	-1083.2	-571.0	-571.1	-1654.3
102	13.15	15.89	-232.18304	-495.5	-1103.6	-468.7	213.5	-1231.2
199	13.21	16.21	-232.17393	-471.8	-1086.8	261.5	-480.6	-1196.4
213	5.33	14.27	-232.11059	-1153.5	-88.3	-1082.4	-1212.3	-1165.7
187	13.58	16.24	-232.05951	-404.6	-1030.1*	524.2	-1091.3	-646.7
185	13.65	16.11	-232.05288	-430.3	-1098.4	-1162.6	-700.8	572.4

*For isomer **187** we do not recover a magnetizability anisotropy larger than benzene, as claimed in ref.¹

References

- (1) Janda, T.; Foroutan-Nejad, C. *ChemPhysChem* **2018**, *19*, 2357–2363.
- (2) Dinadayalane, T. C.; Priyakumar, U. D.; Sastry, G. N. *J. Phys. Chem. A* **2004**, *108*, 11433–11448.